LOW TEMPERATURE XRD INVESTIGATION OF SOLID C_{60} INTERCALATED BY nH_2

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The C_{60} crystal has octahedral and tetrahedral cavities large enough (effective radii are 2.26 and 1.13 Å respectively [1-3,4]) to accommodate various atoms and smaller molecules. For atomic and molecular impurities, the filling may reach values of 60-100%. Under these conditions, an essential influence of the impurities on the structural and thermodynamic characteristics of the C_{60} matrix can appear. Recent work [5] asserts that He, Ne, Ar atoms in the C_{60} lattice are in a bound state and form stoichiometric complexes with C_{60} molecules. These assumptions are not evident and or consistent with simple concepts of impurities.

The influence of intercalation by hydrogen under ambient pressure and temperature on the structure, phase transitions and lattice parameters of fullerite C_{60} has been investigated by X-ray powder diffraction. Because of their small size H_2 molecules fill comparatively easily interstitial spaces of the crystal. The investigation was performed on polycrystalline C_{60} with 99.98% purity. Temperature dependence of the lattice parameters was studied on a hydrogen saturated specimen in the temperature range of 11-295 K (fig 2). The intercalation was proceeding for more than 1000 hours at room temperature and atmospheric pressure. An essential brightening of the structure and superstructure lines in the C_{60} diffraction pattern at temperature below 60 K has been observed (fig. 3). The appearance of new lines at low temperatures is likely to be due to hydrogen influence on the character and degree of the orientation order of C_{60} molecules. Qualitative analysis of the influence of hydrogen in octahedral cavities on the reflection intensities at low temperatures has been performed. It is found that hydrogen intercalation does not entail lattice parameter changes within the sensitivity of the method employed (fig 1). Nevertheless, hydrogen intercalation leads to a noticeable shift to lower temperatures of the orientational *fcc-sc* phase transition (fig 2).

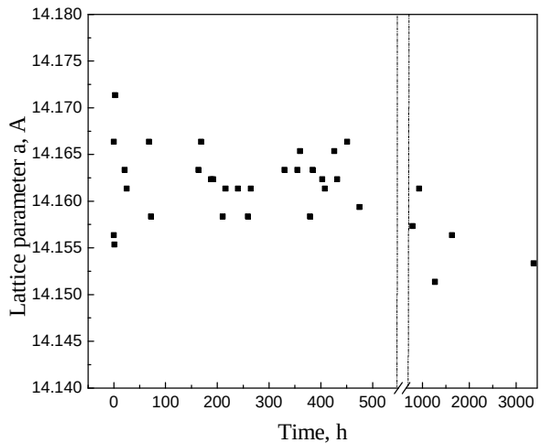

Fig 1 Dependence of the lattice parameters on the intercalation time

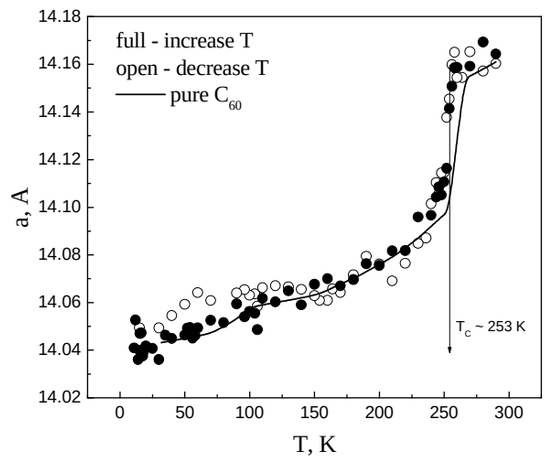

Fig 2 Temperature dependence of the lattice parameters for hydrogen saturated and pure specimens

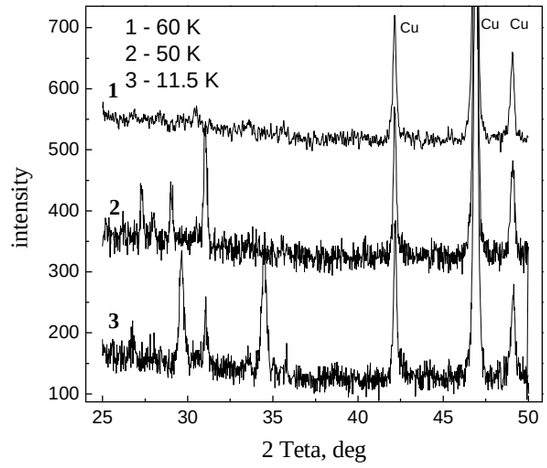

Fig 3 Low temperature XRD pattern of hydrogen-saturated C_{60}. Note the clearly seen brightening of the lines

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